Quantum Entanglement:
Criteria and Collective Tests

Asher Peres*

Department of Physics, Technion—Israel Institute of Technology, 32 000 Haifa, Israel

Abstract

The state of a quantum system, consisting of two distinct subsystems, is called *separable* if it can be prepared by two distant experimenters who receive instructions from a common source, via classical communication channels. A necessary condition is derived and is shown to be more sensitive than Bell's inequality for detecting quantum inseparability. Moreover, collective tests of Bell's inequality (namely, tests that involve several composite systems simultaneously) may sometimes lead to a violation of Bell's inequality, even if the latter is satisfied when each composite system is tested separately.

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* Electronic address: peres@photon.technion.ac.il

1. Introduction

Quantum entanglement is a physical resource. Applications include secure communication between distant observers [1], faithful teleportation of an unknown quantum state to an unknown location [2], quantum computation, and in particular error correction codes [3]. Quantum entanglement is subtler than classical correlation. A composite quantum system can be prepared in a prescribed state ρ, with distant correlations, by two observers who only use local raw materials and receive instructions from a common source by a classical communication channel. Such a preparation method yields a density matrix which is *separable* into a sum of direct products,

$$\rho = \sum_K w_K \, \rho'_K \otimes \rho''_K, \tag{1}$$

where the positive weights w_K satisfy $\sum w_K = 1$, and where ρ'_K and ρ''_K are density matrices for the two subsystems. A separable system represented by the above ρ is *correlated*, but it is not *entangled*: it always satisfies Bell's inequality [4].

That inequality was originally derived for solving a completely different problem: is quantum theory compatible with an underlying pseudo-classical "subquantum" background (deterministic or possibly stochastic)? Such a post-quantum theory would presumably involve additional "hidden" variables, and the statistical predictions of ordinary quantum theory would be reproduced by performing suitable averages over these hidden variables. Bell [4] was the first to show that if the constraint of *locality* is imposed on the hidden variables (namely, if the hidden variables of two distant quantum systems are themselves separable into two distinct subsets), then there is an upper bound to the correlations of results of measurements that can be performed on the two distant systems. That bound is violated by some states in quantum mechanics, for example the singlet state of two spin-$\frac{1}{2}$ particles. It is not quantum theory itself which is nonlocal. It is any pseudo-classical theory which attempts to mimic quantum effects that is necessarily nonlocal and contextual.

A variant of Bell's inequality, more general and more useful for experimental tests, was derived by Clauser, Horne, Shimony, and Holt (CHSH) [5]. It can be written

$$|\langle AB\rangle + \langle AB'\rangle + \langle A'B\rangle - \langle A'B'\rangle| \leq 2. \tag{2}$$

On the left hand side, A and A' are two operators that can be measured by an observer, conventionally called Alice. These operators do not commute (so that Alice has to choose

whether to measure A or A') and each one is normalized to unit norm (the norm of an operator is defined as the largest absolute value of any of its eigenvalues). Likewise, B and B' are two normalized noncommuting operators, any one of which can be measured by another, distant observer (Bob). Note that each one of the *expectation* values in Eq. (2) can be calculated by means of quantum theory, if the quantum state is known, and it is also experimentally observable, by repeating the measurements sufficiently many times, starting each time with identically prepared pairs of quantum systems. The validity of the CHSH inequality, for *all* combinations of measurements independently performed on both systems, is a necessary condition for the possible existence of a local hidden variable (LHV) model for the results of these measurements. It is not in general a sufficient condition, as will be shown below.

Note that, in order to test Bell's inequality, the two distant observers independently *measure* subsytems of a composite quantum system, and then they *report* their results to a common site where that information is analyzed [6]. This is the converse of the situation that was mentioned above, where the two observers *received* instructions from a common center. There are density matrices for which it can be proved that no such set of instructions exists, and yet Bell's inequality is satisfied [7–10]. I shall derive below a simple algebraic test which is a necessary condition for the existence of the decomposition (1). I shall then give some examples showing that this new criterion is more restrictive than Bell's inequality, or than the α-entropy inequality [11].

2. Separability of density matrices

The derivation of the separability condition is easiest when the density matrix elements are written explicitly, with all their indices [6]. For example, Eq. (1) becomes

$$\rho_{m\mu,n\nu} = \sum_K w_K\, (\rho'_K)_{mn}\, (\rho''_K)_{\mu\nu}. \tag{3}$$

Latin indices refer to the first subsystem, Greek indices to the second one (the subsystems may have different dimensions). Note that this equation can always be satisfied if we replace the quantum density matrices by classical Liouville functions (and the discrete indices are replaced by canonical variables, $\mathbf{p}$ and $\mathbf{q}$). The reason is that the only constraint that a Liouville function has to satisfy is being non-negative. On the other hand, we want quantum density matrices to have non-negative *eigenvalues*, rather than non-negative elements, and the latter condition is more difficult to satisfy.

It is noteworthy that any set of instructions that Alice and Bob may receive is inherently ambiguous, if these observers have no way of ascertaining that what one of them calls $i = \sqrt{-1}$ is the same as i (not $-i$) of the other observer. Indeed, the only way of explaining to someone what i and $-i$ actually are is by referring to a material (chiral) object, such as a screw. If we are restricted to the use of verbal instructions for preparing ρ, the result may be either ρ or $\rho^* = \rho^T$. Therefore Alice and Bob may also end up with the "dual" matrix

$$\sigma = \sum_A w_A \, (\rho'_A)^T \otimes \rho''_A. \tag{4}$$

This ambiguity is an important clue for solving the following problem. Let all the matrix elements of ρ be given. Is a decomposition such as in Eq. (1) possible? A simple condition is readily obtained by defining a new matrix,

$$\sigma_{m\mu,n\nu} \equiv \rho_{n\mu,m\nu}. \tag{5}$$

The Latin indices of ρ have been transposed, but not the Greek ones. This is not a unitary transformation but, nevertheless, the σ matrix is Hermitian. Whenever Eq. (1) is valid, the transposed matrices $(\rho'_A)^T \equiv (\rho'_A)^*$ are non-negative matrices with unit trace, so that they also are legitimate density matrices. It follows that *none of the eigenvalues of σ is negative*. This is a necessary condition for Eq. (1) to hold [12].

Note that the eigenvalues of σ are invariant under separate unitary transformations, U' and U'', of the bases used by the two observers. In such a case, ρ transforms as

$$\rho \to (U' \otimes U'') \, \rho \, (U' \otimes U'')^\dagger, \tag{6}$$

and we then have

$$\sigma \to (U'^T \otimes U'') \, \sigma \, (U'^T \otimes U'')^\dagger, \tag{7}$$

which also is a unitary transformation, leaving the eigenvalues of σ invariant.

As an example, consider a pair of spin-$\frac{1}{2}$ particles in an impure singlet state, consisting of a singlet fraction x and a random fraction $(1-x)$ [13]. Note that the "random fraction" $(1-x)$ also includes singlets, mixed in equal proportions with the three triplet components. We have

$$\rho_{m\mu,n\nu} = x \, S_{m\mu,n\nu} + (1-x) \, \delta_{mn} \, \delta_{\mu\nu} \, /4, \tag{8}$$

where the density matrix for a pure singlet is given by

$$S_{01,01} = S_{10,10} = -S_{01,10} = -S_{10,01} = \tfrac{1}{2}, \tag{9}$$

and all the other components of S vanish. (The indices 0 and 1 refer to any two orthogonal states, such as "up" and "down.") A straightforward calculation shows that σ has three eigenvalues equal to $(1+x)/4$, and the fourth eigenvalue is $(1-3x)/4$. This lowest eigenvalue is positive if $x < \frac{1}{3}$, and the separability criterion is then fulfilled. This result may be compared with other criteria: Bell's inequality holds for $x < 1/\sqrt{2}$, and the α-entropic inequality [11] for $x < 1/\sqrt{3}$. These are therefore much weaker tests for detecting inseparability than the condition that was derived here.

In this particular case, it happens that this necessary condition is also a sufficient one. It is indeed known that if $x < \frac{1}{3}$ it is possible to write ρ as a mixture of unentangled product states [14]. This suggests that the necessary condition derived above (σ has no negative eigenvalue) might also be sufficient for any ρ. A proof of this conjecture was indeed recently obtained [15] for composite systems having dimensions 2×2 and 2×3. However, for higher dimensions, the present necessary condition is *not* a sufficient one. Some counterexamples have been constructed, with dimensions 2×4 and 3×3 [16]. It was also shown [16] that the decomposition of any separable ρ requires at most $(\dim \mathcal{H})^2$ terms of rank one. This property is an important step toward finding an *efficient* algorithm for the decomposition of any separable ρ. Such an algorithm, which could also indicate that ρ is not separable, is still lacking at the time of writing.

As a second example, consider a mixed state consisting of a fraction x of the pure state $a|01\rangle + b|10\rangle$ (with $|a|^2 + |b|^2 = 1$), and fractions $(1-x)/2$ of the pure states $|00\rangle$ and $|11\rangle$. We have

$$\rho_{00,00} = \rho_{11,11} = (1-x)/2, \tag{10}$$

$$\rho_{01,01} = x|a|^2, \tag{11}$$

$$\rho_{10,10} = x|b|^2, \tag{12}$$

$$\rho_{01,10} = \rho^*_{10,01} = xab^*, \tag{13}$$

and the other elements of ρ vanish. It is easily seen that the σ matrix has a negative determinant, and thus a negative eigenvalue, when

$$x > (1 + 2|ab|)^{-1}. \tag{14}$$

This is a lower limit than the one for a violation of Bell's inequality, which requires [10]

$$x > [1 + 2|ab|(\sqrt{2} - 1)]^{-1}. \tag{15}$$

An even more striking example is the mixture of a singlet and a maximally polarized pair:

$$\rho_{m\mu,n\nu} = x\, S_{m\mu,n\nu} + (1 - x)\, \delta_{m0}\, \delta_{n0}\, \delta_{\mu0}\, \delta_{\nu0}. \tag{16}$$

For any positive x, however small, this state is inseparable, because σ has a negative eigenvalue $(-x/2)$. On the other hand, the Horodecki criterion [17] gives a very generous domain to the validity of Bell's inequality: $x \leq 0.8$.

3. Collective tests for nonlocality

The weakness of Bell's inequality as a test for inseparability is due to the fact that the only use made of the density matrix ρ is for computing the probabilities of the various outcomes of tests that may be performed on the subsystems of a *single* composite system. On the other hand, an experimental verification of that inequality necessitates the use of *many* composite systems, all prepared in the same way. However, if many such systems are actually available, we may also test them collectively, for example two by two, or three by three, etc., rather than one by one. If we do that, we must use, instead of ρ (the density matrix of a single system), a *new* density matrix, which is $\rho \otimes \rho$, or $\rho \otimes \rho \otimes \rho$, in a higher dimensional space. It will now be shown that there are some density matrices ρ that satisfy Bell's inequality, but for which $\rho \otimes \rho$, or $\rho \otimes \rho \otimes \rho$, etc., violate that inequality [18].

The example that will be discussed is that of the Werner states [7] defined by Eq. (8). Let us consider n Werner pairs. Each one of the two observers has n particles (one from each pair). They proceed as follows. First, they subject their n-particle systems to suitably chosen local unitary transformations, U, for Alice, and V, for Bob. Then, they test whether each one of the particles labelled 2, 3, …, n, has spin up (for simplicity, it is assumed that all the particles are distinguishable, and can be labelled unambiguously). Note that any other test that they can perform is unitarily equivalent to the one for spins up, as this involves only a redefinition of the matrices U and V. If any one of the $2(n-1)$ particles tested by Alice and Bob shows spin down, the experiment is considered to have failed, and the two observers must start again with n new Werner pairs.

A similar elimination of “bad” samples is also inherent to any experimental procedure where a failure of one of the detectors to fire is handled by discarding the results registered by all the other detectors: only when *all* the detectors fire are their results included in the statistics. This obviously requires an exchange of *classical* information between the observers. (There is a controversy on whether a violation of Bell’s inequality with postselected data [19] is a valid test for nonlocality [20]. I shall not discuss this issue here; I only examine whether or not Bell’s inequality is violated by the postselected data.)

The calculations shown below will refer to the case $n = 3$, for definiteness. The generalization to any other value of n is straightforward. Spinor indices, for a single spin-$\frac{1}{2}$ particle, will take the values 0 (for the “up” component of spin) and 1 (for the “down” component). The 16 components of the density matrix of a Werner pair, consisting of a singlet fraction x and a random fraction $(1-x)$, are, in the standard direct product basis:

$$\rho_{mn,st} = x\, S_{mn,st} + (1-x)\, \delta_{ms}\, \delta_{nt}\, /4, \tag{17}$$

where I am now using only Latin indices, contrary to what I did in Eq. (8); this is because Greek indices will be needed for another purpose, as will be seen soon. Thus, now, the indices m and s refer to Alice’s particle, and n and t to Bob’s particle.

When there are three Werner pairs, their combined density matrix is a direct product $\rho\otimes\rho'\otimes\rho''$, or explicitly, $\rho_{mn,st}\, \rho_{m'n',s't'}\, \rho_{m''n'',s''t''}$. The result of the unitary transformations U and V is

$$\rho \otimes \rho' \otimes \rho'' \to (U \otimes V)\, (\rho \otimes \rho' \otimes \rho'')\, (U^\dagger \otimes V^\dagger). \tag{18}$$

Explicitly, with all its indices, the U matrix satisfies the unitarity relation

$$\sum_{mm'm''} U_{\mu\mu'\mu'',mm'm''}\, U^*_{\lambda\lambda'\lambda'',mm'm''} = \delta_{\mu\lambda}\, \delta_{\mu'\lambda'}\, \delta_{\mu''\lambda''}. \tag{19}$$

In order to avoid any possible ambiguity, Greek indices (whose values are also 0 and 1) are now used to label spinor components *after* the unitary transformations. Note that the indices without primes refer to the two particles of the first Werner pair (the only ones that are not tested for spin up) and the primed indices refer to all the other particles (that are tested for spin up). The $V_{\nu\nu'\nu'',nn'n''}$ matrix elements of Bob’s unitary transformation satisfy a relationship similar to (19). The generalization to a larger number of Werner pairs is obvious.

After the execution of the unitary transformation (18), Alice and Bob have to test that all the particles, except those labelled by the first (unprimed) indices, have their

spin up. They discard any set of n Werner pairs where that test fails, even once. The density matrix for the remaining "successful" cases is thus obtained by retaining, on the right hand side of Eq. (18), only the terms whose primed components are zeros, and then renormalizing the resulting matrix to unit trace. This means that only two of the 2^n rows of the U matrix, namely those with indices 000... and 100..., are relevant (and likewise for the V matrix). The elimination of all the other rows greatly simplifies the problem of optimizing these matrices. We shall thus write, for brevity,

$$U_{\mu 00,mm'm''} \to U_{\mu,mm'm''}, \tag{20}$$

where $\mu = 0, 1$. Then, on the left hand side of Eq. (19), we effectively have two unknown row vectors, U_0 and U_1, each one with 2^n components (labelled by Latin indices $mm'm''$). These vectors have unit norm and are mutually orthogonal. Likewise, Bob has two vectors, V_0 and V_1. The problem is to optimize these four vectors so as to make the expectation value of the Bell operator [21],

$$C := AB + AB' + A'B - A'B', \tag{21}$$

as large as possible.

The optimization proceeds as follows. The new density matrix, for the pairs of spin-$\frac{1}{2}$ particles that were *not* tested by Alice and Bob for spin up (that is, for the first pair in each set of n pairs), is

$$(\rho_{\rm new})_{\mu\nu,\sigma\tau} = N\, U_{\mu,mm'm''}\, V_{\nu,nn'n''}\, \rho_{mn,st}\, \rho_{m'n',s't'}\, \rho_{m''n'',s''t''}\, U^*_{\sigma,ss's''}\, V^*_{\tau,tt't''}, \tag{22}$$

where N is a normalization constant, needed to obtain unit trace (N^{-1} is the probability that all the "spin up" tests were successful). We then have [17], for fixed $\rho_{\rm new}$ and all possible choices of C,

$$\max\left[{\rm Tr}\,(C\rho_{\rm new})\right] = 2\sqrt{M}, \tag{23}$$

where M is the sum of the two largest eigenvalues of the real symmetric matrix $T^\dagger T$, defined by

$$T_{pq} := {\rm Tr}\left[(\sigma_p \otimes \sigma_q)\,\rho_{\rm new}\right]. \tag{24}$$

(In the last equation, σ_p and σ_q are the Pauli spin matrices.) Our problem is to find the vectors U_μ and V_ν that maximize M.

At this point, some simplifying assumptions are helpful. Since all matrix elements $\rho_{mn,st}$ are real, it is reasonable to restrict the search to vectors U_μ and V_ν that have only real components. Furthermore, the situations seen by Alice and Bob are completely symmetric, except for the opposite signs in the standard expression for the singlet state:

$$\psi = \left[\binom{1}{0}\binom{0}{1} - \binom{0}{1}\binom{1}{0}\right] /\sqrt{2}. \tag{25}$$

These signs can be made to become the same by redefining the basis, for example by representing the "down" state of Bob's particle by the symbol $\binom{0}{-1}$, *without* changing the basis used for Alice's particle. This unilateral change of basis is equivalent a substitution

$$V_{\nu,nn'n''} \to (-1)^{\nu+n+n'+n''}\, V_{\nu,nn'n''}, \tag{26}$$

on Bob's side. The minus signs in Eq. (9) also disappear, and there is complete symmetry for the two observers. It is then plausible that, with the new basis, the optimal U_ν and V_ν are the same. Therefore, when we return to the original basis and notations, they satisfy

$$V_{\nu,nn'n''} = (-1)^{\nu+n+n'+n''}\, U_{\nu,nn'n''}. \tag{27}$$

We shall henceforth restrict our search to pairs of vectors that satisfy this relation.

After all the above simplifications, the problem that has to be solved is the following: find two mutually orthogonal unit vectors, U_0 and U_1, each one with 2^n real components, that maximize the value of $M(U)$ defined by Eqs. (23) and (24). This is a standard optimization problem which can be solved numerically. Since the function $M(U)$ is bounded, it has at least one maximum. It may, however, have more than one: there may be several distinct local maxima with different values. A numerical search leads to one of these maxima, but not necessarily to the largest one. The outcome may depend on the initial point of the search. It is therefore imperative to start from numerous randomly chosen points in order to ascertain, with reasonable confidence, that the largest maximum has indeed been found.

4. Numerical results

In all the cases that were examined, $M(U)$ turned out to have a local maximum for the following simple choice:

$$U_{0,00\ldots} = U_{1,11\ldots} = 1, \tag{28}$$

and all the other components of U_0 and U_1 vanish. Recall that the "vectors" U_0 and U_1 actually are two rows, $U_{000\ldots}$ and $U_{100\ldots}$, of a unitary matrix of order 2^n (the other rows are irrelevant because of the elimination of all the experiments in which a particle failed the spin-up test). In the case $n = 2$, one of the unitary matrices having the property (28) is a simple permutation matrix that can be implemented by a "controlled-NOT" quantum gate [22] known as XOR (exclusive OR). For larger values of n, matrices that satisfy Eq. (28) will also be called XOR-transformations.

It was found, by numerical calculations, that XOR-transformations always are the optimal ones for $n = 2$. They are also optimal for $n = 3$ when the singlet fraction x is less than 0.57, and for $n = 4$ when $x < 0.52$. For larger values of x, more complicated forms of U_0 and U_1 give better results. For $n = 3$, it was recently found that the optimum is a "controlled Hadamard transform"

$$U_{0,000} = U_{0,111} = U_{1,001} = U_{1,100} = 1/\sqrt{2}. \tag{29}$$

The corresponding result for higher n is not known. Anyway, the existence of two different sets of maxima may be seen in Fig. 1: there are discontinuities in the slopes of the graphs for $n = 3$ and 4, that occur at the values of x where the largest value of $\langle C \rangle$ jumps from one local maximum to another one.

For $n = 5$, a complete determination of U_0 and U_1 requires the optimization of 64 parameters subject to 3 constraints, more than my workstation could handle in a reasonable time. I therefore considered only XOR-transformations, which are likely to be optimal for $x \lesssim 0.5$. In particular, for $x = 0.5$ (the value that was used in Werner's original work [7]), the result is $\langle C \rangle = 2.0087$, and the CHSH inequality is violated. This violation occurs in spite of the existence of an explicit LHV model that gives correct results if the Werner pairs are tested one by one.

These results prompt a new question: can we get stronger *inseparability* criteria by considering $\rho \otimes \rho$, or higher tensor products? It is easily seen that no further progress can be achieved in this way. If ρ is separable as in Eq. (1), so is $\rho \otimes \rho$. Moreover, the partly transposed matrix corresponding to $\rho \otimes \rho$ simply is $\sigma \otimes \sigma$, so that if no eigenvalue of σ is negative, then $\sigma \otimes \sigma$ too has no negative eigenvalue.

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1. Ekert, A. K., Phys. Rev. Lett. **67**, 661 (1991).

2. Bennett, C. H, Brassard, G., Crépeau, C., Jozsa, R., Peres, A., and Wootters, W. K., Phys. Rev. Lett. **70**, 1895 (1993).

3. Knill, E., and Laflamme, R., Phys. Rev. A **55**, 900 (1997).

4. Bell, J. S., Physics **1**, 195 (1964).

5. Clauser, J. F., Horne, M. A., Shimony, A., and Holt, R. A., Phys. Rev. Lett. **23**, 880 (1969).

6. Peres, A., "Quantum Theory: Concepts and Methods" (Kluwer, Dordrecht, 1993) Chapters 5 and 6.

7. Werner, R. F., Phys. Rev. A **40**, 4277 (1989).

8. Popescu, S., Phys. Rev. Lett. **72**, 797 (1994); **74**, 2619 (1995).

9. Mermin, N. D., in "Perspectives on Quantum Reality" (Edited by R. K. Clifton) (Kluwer, Dordrecht, 1996) pp. 57–71.

10. Gisin, N., Phys. Lett. A **210**, 151 (1996).

11. Horodecki, R., Horodecki, P., and Horodecki, M., Phys. Lett. A **210**, 377 (1996).

12. Peres, A., Phys. Rev. Lett. **77**, 1413 (1996).

13. Blank, J. and Exner, P., Acta Univ. Carolinae, Math. Phys. **18**, 3 (1977).

14. Bennett, C. H., Brassard, G., Popescu, S., Schumacher, B., Smolin, J., and Wootters, W. K., Phys. Rev. Lett. **76**, 722 (1996); **78**, 2031 (1997) (E).

15. Horodecki, M., Horodecki, P., and Horodecki, R., Phys. Lett. A **223**, 1 (1996).

16. Horodecki, P., "Separability criterion and inseparable mixed states with positive partial transposition" (e-print archive: quant-ph/9605038).

17. Horodecki, R., Horodecki, P., and Horodecki, M., Phys. Lett. A **200**, 340 (1995).

18. Peres, A., Phys. Rev. A **54**, 2685 (1996).

19. Peres, A., in "Quantum Potentiality, Entanglement, and Passion-at-a-Distance: Essays for Abner Shimony" (Edited R. S. Cohen, M. Horne, and J. Stachel) (Kluwer, Dordrecht, 1997).

20. Santos, E., Phys. Rev. Lett. **66**, 1388 (1991).

21. Braunstein, S. L., Mann, A., and Revzen, M., Phys. Rev. Lett. **68**, 3259 (1992).

22. Barenco, A., Deutsch, D., Ekert, A., and Jozsa, R., Phys. Rev. Lett. **74**, 4083 (1995).

Caption of figure

FIG. 1. Maximal expectation value of the Bell operator, versus the singlet fraction in the Werner state, for collective tests performed on several Werner pairs (from bottom to top of the figure, 1, 2, 3, and 4 pairs, respectively). The CHSH inequality is violated when $\langle C\rangle > 2$.